Problems in Covariance Evaluations

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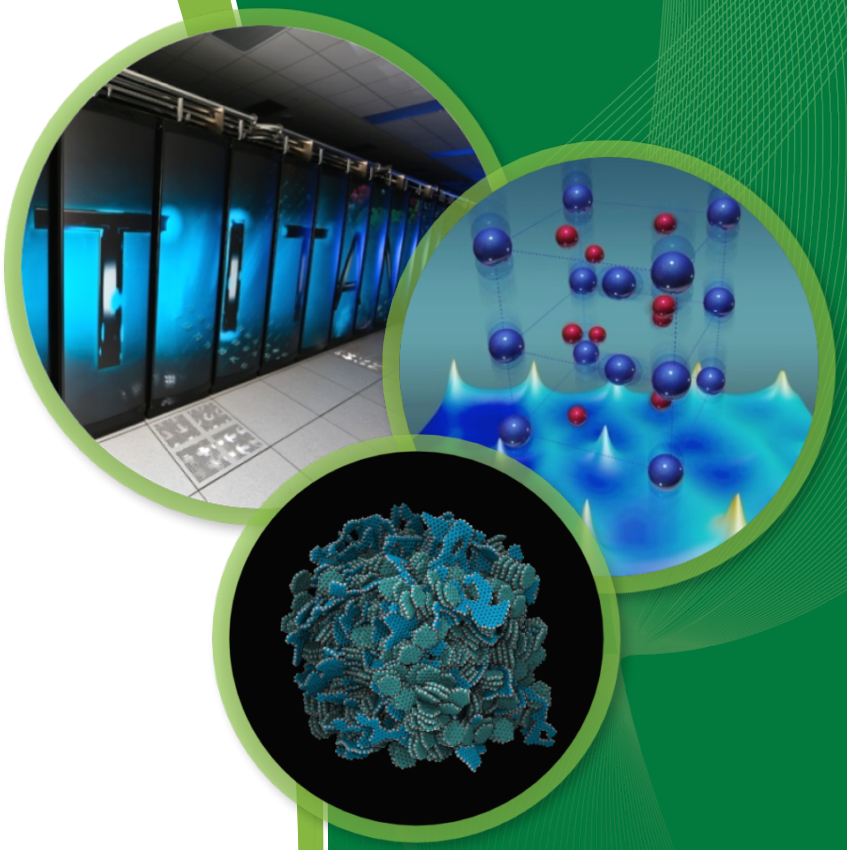

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SCALE-6.2 Covariance Library

- The SCALE-6.2 covariance library includes:
  - ENDF/B-VII.1 for 187 isotopes; SCALE-6.1 data (mainly Lo-Fi) retained for ~215 missing nuclides
  - Modified ENDF/B-VII.1 ^{239}Pu, ^{235}U nubar and H capture uncertainties; these are prerelease ENDF/VIII.0 rev. 632, 631 and 611
  - Chi uncertainties processed from new ENDF/B-VII.1 file 35
  - Chi uncertainties from JENDL4.0 for ^{241}Am, ^{242}Am, ^{243}Am, ^{244}Am, ^{237}Np, ^{231}Pa, ^{233}Pa, ^{241}Pu, ^{232}Th, ^{233}U, ^{234}U, ^{236}U, ^{237}U
  - Updated thermal capture values for ^{255}Eu, ^{147}Pm, ^{103}Rh, ^{149}Sm, ^{151}Sm (to be equal to Atlas values)

SCALE sensitivity tools currently only use the following reactions: 1, 2, 4, 16, 18, 102, 103, 104, 105, 106, 107, 452, 455, 456. Therefore, this presentation concentrates on those reactions

Compare ENDF/B-VIII.0 beta with ENDF/B-VII.1

All comparisons are made with Rev. 1106 from the ENDF svn repository

For comparison with ENDF/B-VII.1 only, ENDF/B-VII.1 point-wise cross section data are used

For all other cases, including the data shown in Marshall's discussion, point-wise cross section data from Rev. 1106 are used

New covariance matrices in ENDF/B-VIII.0 are listed below:

- ^{7}Be
- ^{40}Ca
- ^{63}Cu
- ^{65}Cu
- ^{233}U chi covariance data

Some cross reaction covariance matrices in ^{240}Pu and ^{16}O have also been added

Compare ENDF/B-VIII.0 beta with ENDF/B-VII.1 (continued)

- Covariance data are in ENDF/B-VII.1 but not in ENDF/B-VIII.0 beta
  - Nuclides where **all** covariance data are deleted:
    - ^{6}Li, including cross material matrices with ^{10}B, ^{235}U, and ^{239}Pu
    - ^{10}B, ^{54}Fe, ^{56}Fe, ^{57}Fe, ^{59}Co, ^{239}Pu
  - Nuclides where some covariance data are retained:
    - ^{238}U only kept MT=452, 456 and 18, and oddly, cross reaction [18,102] but no covariance data for [102,102]) and chi
    - ^{235}U only kept MT=452, 455, 456 and chi and cross material covariance data for 452
    - Due to new evaluations, ^{16}O lost covariance data for MT=4, 16, 102, 103, 104, 105, 107 and only contains data for [2,2] and [800,107], which cannot be used without covariance data for 800 and 107
- Several cross material covariances can no longer be calculated

Compare ENDF/B-VIII.0 beta with ENDF/B-VII.1 (continued)

- Differences between the two libraries:
  - ^{16}O, ^{182}W, ^{183}W, ^{184}W, ^{186}W due to new evaluations
  - ^{197}Au, MT=102 due to new evaluations
  - ^{233}U due to new evaluation
  - ^{240}Pu due to retrieving old ORNL File 32 data
- Expected differences that are not found
  - Modified ENDF/B-VII.1 ^{239}Pu, ^{235}U nubar and H capture uncertainties from prerelease ENDF/VIII.0 revs. 632, 631 and 611, respectively
  - Reverted back to the old ENDF/B-VII.1 data in ENDF/B-VIII.0 instead of retaining the fixed versions

Processing of ENDF/B-VIII.0 beta

- Processing errors reported by PUFF:
  - **^{154}Gd:** the same resonance (energy and all widths) is given twice in Files 2 and 32. Since the order of resonance in File 32 does not need to be the same as File 2, this leads to bookkeeping problems
  - **^{7}Li:** Matrix for MT=2 is derived from MT=1, 4, and 851 in range [105 eV, 20 MeV]. This implies many cross reaction matrices, among them [1,2], which should not be given in the ENDF in this range, but it is
  - **^{58}Ni and ^{60}Ni** have covariance data for MT=3, but MT=3 is not given in File 3

Processing of ENDF/B-VIII.0 beta (continued)

- PUFF calculates covariance data for redundant cross sections if they do not exist, even if not implicitly defined in ENDF
- All cross reaction covariances that are implied will also be calculated
  - If any two of MT=452, 455, or 456 exist, the third will be calculated
  - MT=1, 4, and any other redundancies will be calculated

Processing of ENDF/B-VIII.0 beta (continued)

- Nuclides that do not have covariance data for total:

  ^{242m1}Am, ^{243}Am, ^{141}Ce, ^{54}Cr, ^{166}Er, ^{167}Er, ^{168}Er, ^{17}Er, ^{153}Eu, ^{155}Eu, ^{127}I, ^{129}I, ^{139}La, ^{25}Mg, ^{26}Mg, ^{95}Nb, ^{16}O, ^{105}Pd, ^{106}Pd, ^{107}Pd, ^{108}Pd, ^{147}Pm, ^{241}Pu, ^{103}Rh, ^{101}Ru, ^{102}Ru, ^{103}Ru, ^{104}Ru, ^{106}Ru, ^{149}Sm, ^{151}Sm, ^{152}Sm, ^{169}Tm, ^{234}U, ^{236}U, ^{238}U, ^{131}Xe, ^{132}Xe, ^{134}Xe

  – MT=1, 4 and any other redundancies will be calculated

- Nuclides that do not have covariance data for MT=4:

  ^{55}Mn, ^{232}Th, 1^{80}W, ^{183}W, ^{184}W, ^{186}W

  There are covariance data for 51 and lumped reaction data that cover the other discrete inelastic reactions. PUFF currently does not consider lumped reaction in summing of redundant data

- Nuclides that do not have covariance data for MT=455: ^{235}U, ^{238}Pu

Processing of ENDF/B-VIII.0 beta (continued)

Check whether covariance data are available over the whole range for reactions for which covariance information is given

This is done automatically if preparing the final covariance library using AMPX module COGNAC

- PUFF has an option to print all File 31 and File 33 covariance matrices on the evaluator grid
- Some nuclides only have covariance matrices for File 32 (and maybe additional background covariance data in the same range: ^{135}C, ^{137}C, ^{39}K, ^{54}Cr, ^{63}Cu, ^{65}Cu, ^{170}Tm, ^{203}Tl, ^{205}TL, ^{40}Ca
- In addition, ^{169}Tm has MT=16 over its entire range

Processing of ENDF/B-VIII.0 beta (continued)

- ^{41}K total is calculated from File 32 data, but File 33 does not give MT=1
  - ^{237}Np
  - MT=456 covariance data start at 0.1 eV
  - MT=1, 2, 102, and 18 start at 0.0253eV
  - Cross section data start at 1e-5 eV
- Covariance matrices for threshold reaction 4, 106, or 107 start at higher energies than the cross section data: ^{53}Cr (4), ^{58}Ni (107), and all Zr (Mt=4)
- Totals are given for higher energy ranges but not lower ranges: ^{197}Au, ^{94}Zr
- Chi covariance data do not extend to the same lower energies as the chi cross section data: ^{235}U, ^{238}U, ^{238}Pu, ^{240}Pu, ^{233}U

Comparison to Mughabghab's Atlas for thermal data

PUFF is run with one group from 0.0253–0.0254 and 1/E flux to calculate the capture and fission cross section data and uncertainty for comparison with Atlas values

- 140 nuclides have both covariance data and Atlas values for capture
- For 95 of the nuclides, the thermal capture cross section agrees with Atlas values within uncertainty
- Of the 95 nuclides, the following have uncertainty in capture that is more than twice the Atlas value:
  ^{1}H, ^{153}Gd, ^{127}I, ^{208}Pb, ^{19}F, ^{237}Np, ^{243}Cm, ^{155}Gd, ^{151}Sm, ^{129}I, ^{149}Sm, ^{244}Pu, ^{103}Rh, ^{232}Th, ^{41}K, ^{255}Es, and ^{7}L
- Nuclides that have uncertainties in capture less than 0.5 Atlas value: ^{39}K39, and ^{242}Cm

Comparison to Mughabghab's Atlas for thermal data (continued)

- 30 nuclides have both covariance data and Atlas values for fission
- For 22 of these nuclides, the thermal fission cross section agrees with Atlas values within uncertainty.
- Of these 22 nuclides, the following have uncertainty in capture that is more than twice the Atlas value:

  ^{255}Fm, ^{253}Cf, ^{229}Th, ^{233}Th, ^{241}Am, ^{232}Pa, ^{241}Pu, and ^{237}Pu

  Nuclides that have uncertainties in capture less than 0.5 Atlas value: ^{236}Pu, ^{248}Cm, and ^{252}Cf

Comparison to Mughabghab's Atlas for resonance integral data

PUFF is run with one group from 0.5–2e7 and 1/E flux to calculate capture and fission cross section data, multiply by group-averaged flux, and compare with Atlas values

- 118 nuclides contain both Atlas values and covariance data for the capture integral
- For 63 of these nuclides, the capture integral value agrees with the Atlas uncertainty
- For 26 of these nuclides, the capture integral value agrees with twice the Atlas uncertainty
- Of the 63 nuclides for which the capture integral agrees, the following have an uncertainty in the capture integral twice as large as the Atlas value: ^{254}Es, ^{108}Pd, ^{247}Cm, ^{242}Pu, ^{250}Cf, ^{131}Xe, ^{243}Cm. ^{23}Na, ^{245}Cm, ^{127}I, ^{244}Cm
- From the 26 nuclides where the capture integral value agrees within the Atlas uncertainty, the following have an uncertainty in the capture integral twice as large as the Atlas value: ^{147}Pm, ^{249}Cf, ^{246}Cm

Summary

- ENDF/B-VIII.0 beta data are processed with PUFF and COGNAC and compared with ENDF/B-VII.1
- All warnings issued by PUFF are evaluated
- COGNAC is run to prepare the covariance library for SCALE, including a check for partial range covariance data
- Thermal capture and fission uncertainties are compared with Mughabghab's Atlas values
- Resonance integral uncertainties for capture and fission are compared with Mughabghab's Atlas values
- Two SCALE libraries are prepared
  - One containing only ENDF/B-VIII.0 beta covariance data
  - Second one adds SCALE 6.2 covariance matrices not already on the ENDF/B-VIII.0 beta covariance library are added
- Tests of these libraries are discussed in Marshall's presentation